

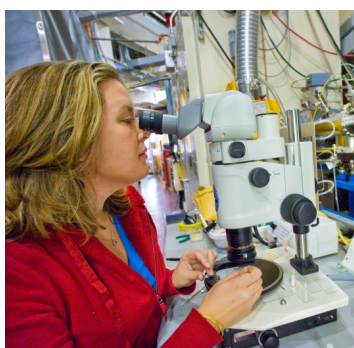
Christine M. Beavers, Ph.D., Chemistry

Years of Fellowship: 2009-2012

Collaborating Institution: University of California, Davis

Currently: ALS

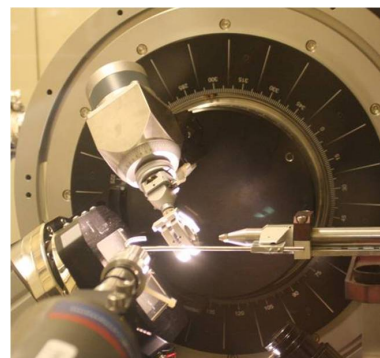
Project: Fullerene structure determination and high pressure chemical crystallography



As an ALS Postdoctoral Fellow, Christine Beavers helped develop two primary fields of research: fullerene structure determination and high pressure chemical crystallography.

Fullerenes are cage compounds, sometimes with atoms inside, composed of five- and six-membered rings of carbon atoms. Data collection on fullerene crystals had previously been an onerous task, involving multiple day data collections on home lab sources that rarely allowed high-resolution refinements. Past attempts to use synchrotron radiation to improve the outcome had been foiled by the use of protein crystallography beamlines, which were not appropriately equipped for inorganic compounds. Through careful analysis of the pitfalls of collecting data on such highly disordered systems, and some trial and error, Christine completed many successful data collections on fullerene compounds. The ensuing refinement of highly disordered fullerenes requires patience, dedication, and a thorough understanding of fullerene chemistry. One extremely difficult case was $\text{Gd}_3\text{N}@C_{78}$ (Beavers, et al., JACS, 2009), which suffered from rotational and racemic disorder; this structure took three months to achieve a satisfactory refinement. This and seven other high-profile fullerene publications have cemented 11.3.1 as a major player worldwide in fullerene crystallography. The Balch and Olmstead group, from UC Davis, continue to use 11.3.1, and to collaborate closely with Christine. This collaboration now extends to groups from Clemson, Virginia Tech, Southern Mississippi, and others.

High pressure crystallography has been used by geologists for decades, but only recently have chemists discovered its great utility in triggering chemical reactions and phase changes. The experiment is technically very challenging and time consuming, but the resulting information, especially material properties such as stress and strain relationships, can be enlightening. A crystal of a magnetic complex that was known to undergo a pressure-induced spin transition was placed into the diamond anvil cell, and subjected to 3GPa of pressure. The spin change was clearly noted in the altered bond lengths, and with this positive outcome, the high-pressure program on 11.3.1 began in earnest. The samples have become more varied, and now include metal organic frameworks, which have numerous potential applications including gas separation and CO_2



storage. Unfortunately, high pressure experiments are still limited by the flux available at higher energies on 11.3.1, but this will be alleviated by a planned move of this program to a superbend beamline.

Christine continues her work on fullerenes, high pressure crystallography and other complicated crystallographic systems on 11.3.1, as a project scientist. The skills she has developed as an ALS Postdoctoral Fellow are invaluable to users; any encountered crystallographic difficulty becomes Christine's next invigorating challenge. Christine is also now involved in the development of pump-probe capability on 11.3.1, and single-crystal high pressure diffraction on beamline 12.2.2. She is also active in publicizing 11.3.1's capabilities, and recruiting new users.

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